wwPDB X-ray Structure Validation Summary Report (i)

Jun 17, 2024 – 12:15 AM EDT

PDB ID	:	5MSR
Title	:	Structure of the unmodified PCP-R domain of carboxylic acid reductase (CAR) from Segniliparus rugosus in complex with NADPH, P43 form
Authors	:	Gahloth, D.; Leys, D.
Deposited on	:	2017-01-05
Resolution	:	2.37 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

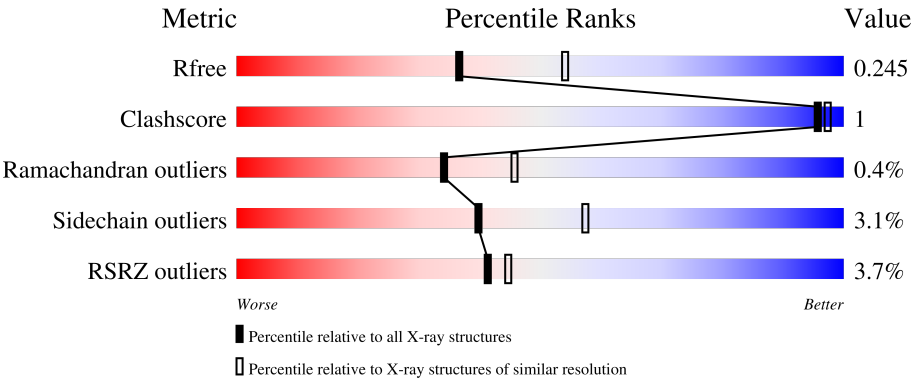
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1188	41% · 57%
1	B	1188	42% · 56%
1	C	1188	41% · · 57%
1	D	1188	40% · 58%

2 Entry composition (i)

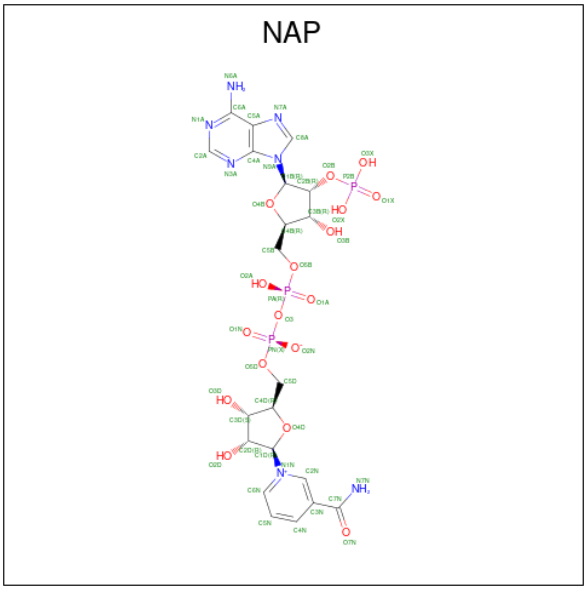
There are 3 unique types of molecules in this entry. The entry contains 16105 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Thioester reductase domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			3926	2492	687	746	1			
1	B	520	Total	C	N	O	S	0	0	0
			3973	2519	693	760	1			
1	C	516	Total	C	N	O	S	0	0	0
			3944	2504	689	750	1			
1	D	504	Total	C	N	O	S	0	0	0
			3869	2461	676	731	1			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			40	15	6	16	3		
2	B	1	Total	C	N	O	P	0	0
			40	15	6	16	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			40	15	6	16	3		
2	D	1	Total	C	N	O	P	0	0
			40	15	6	16	3		

- Molecule 3 is water.

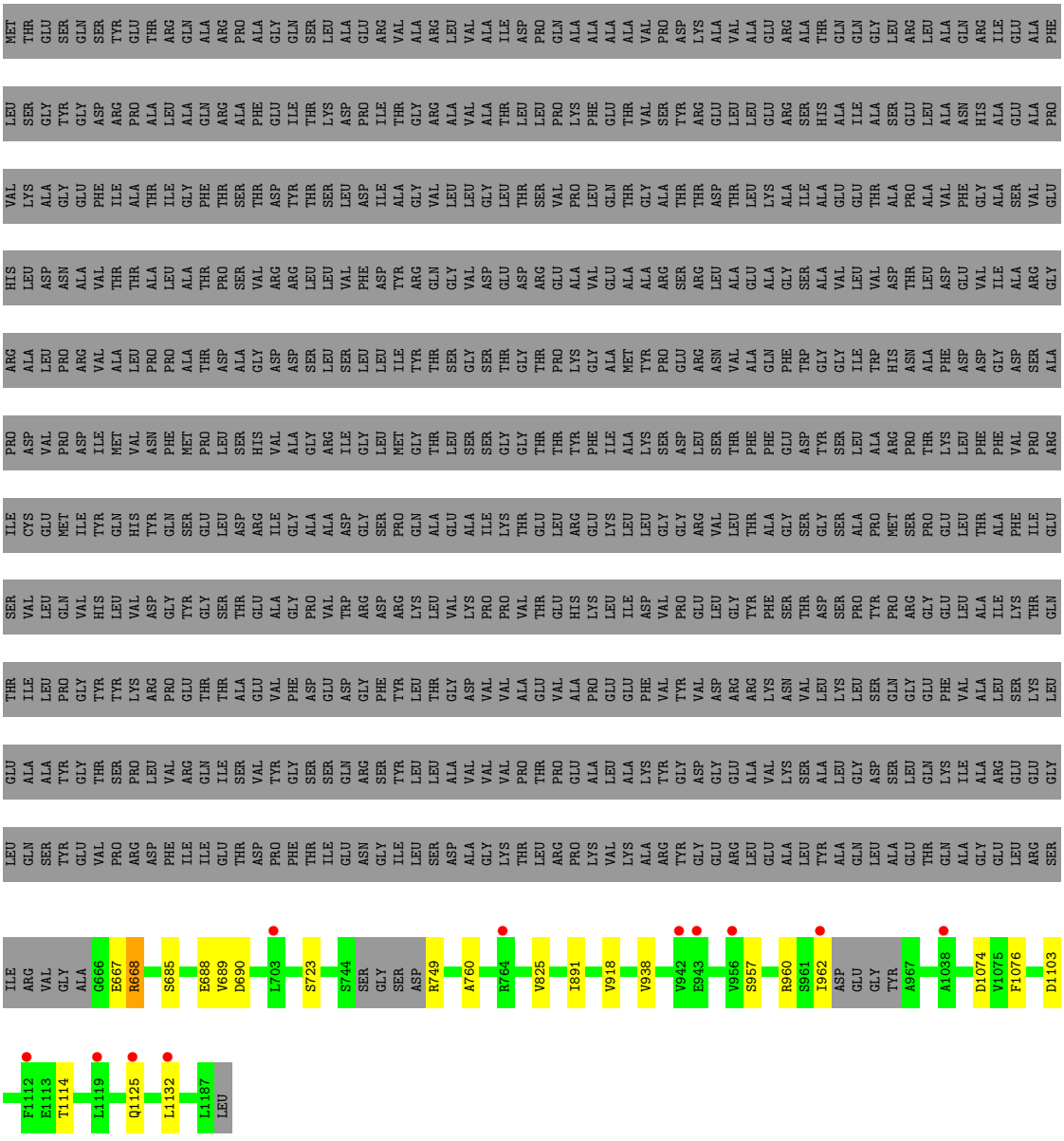
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	63	Total	O	0	0
			63	63		
3	B	75	Total	O	0	0
			75	75		
3	C	58	Total	O	0	0
			58	58		
3	D	37	Total	O	0	0
			37	37		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

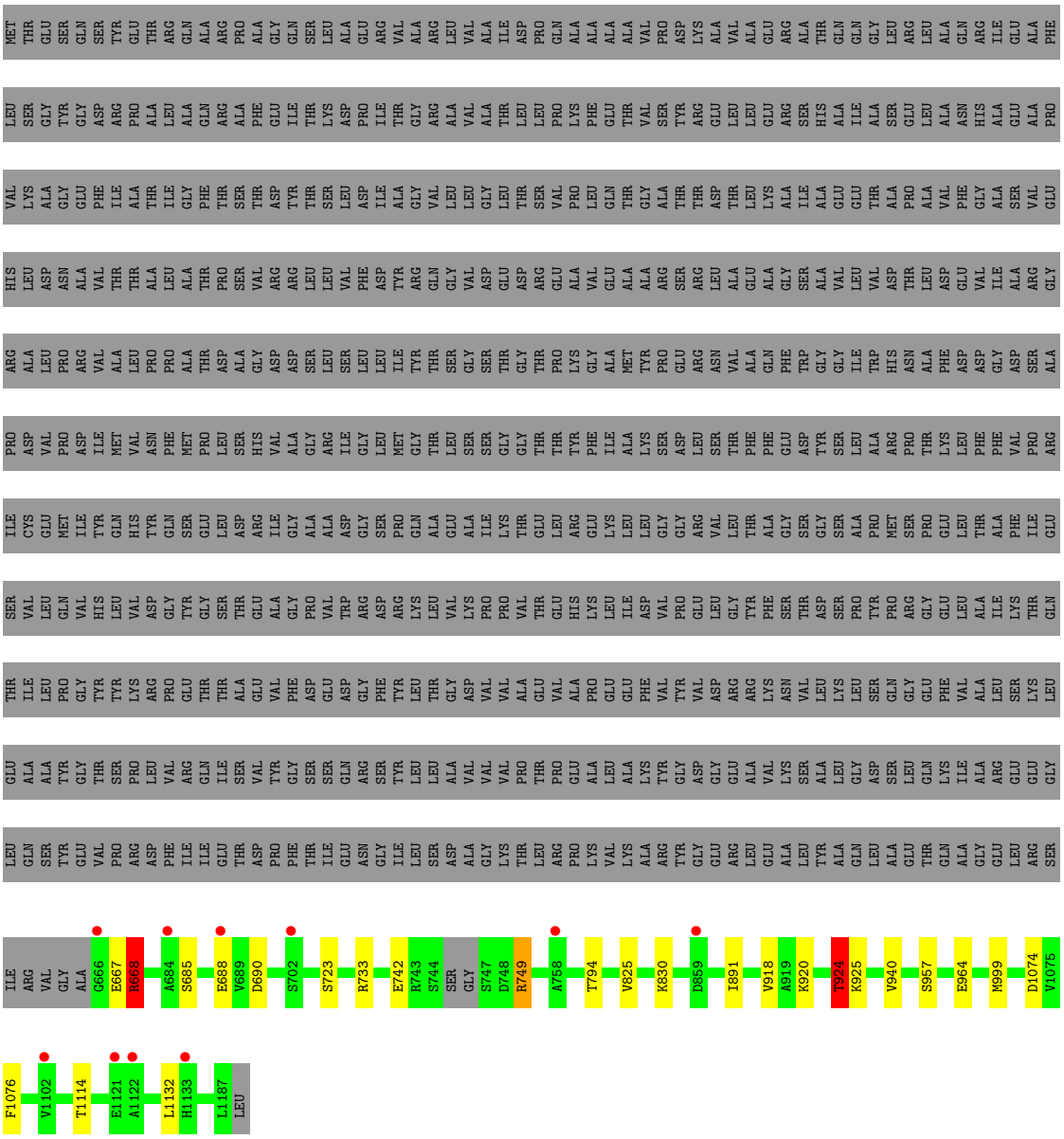
• Molecule 1: Thioester reductase domain-containing protein

Chain A:



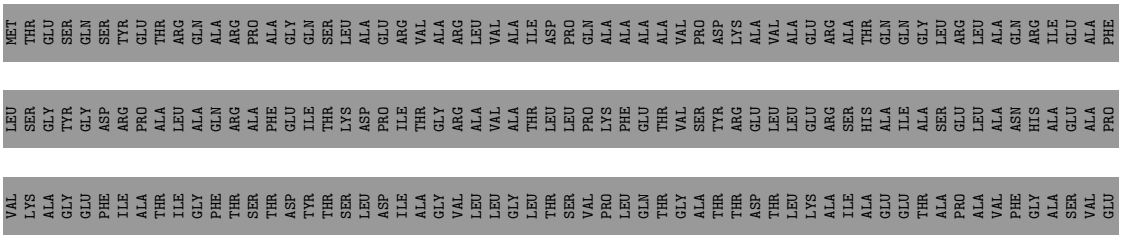
• Molecule 1: Thioester reductase domain-containing protein

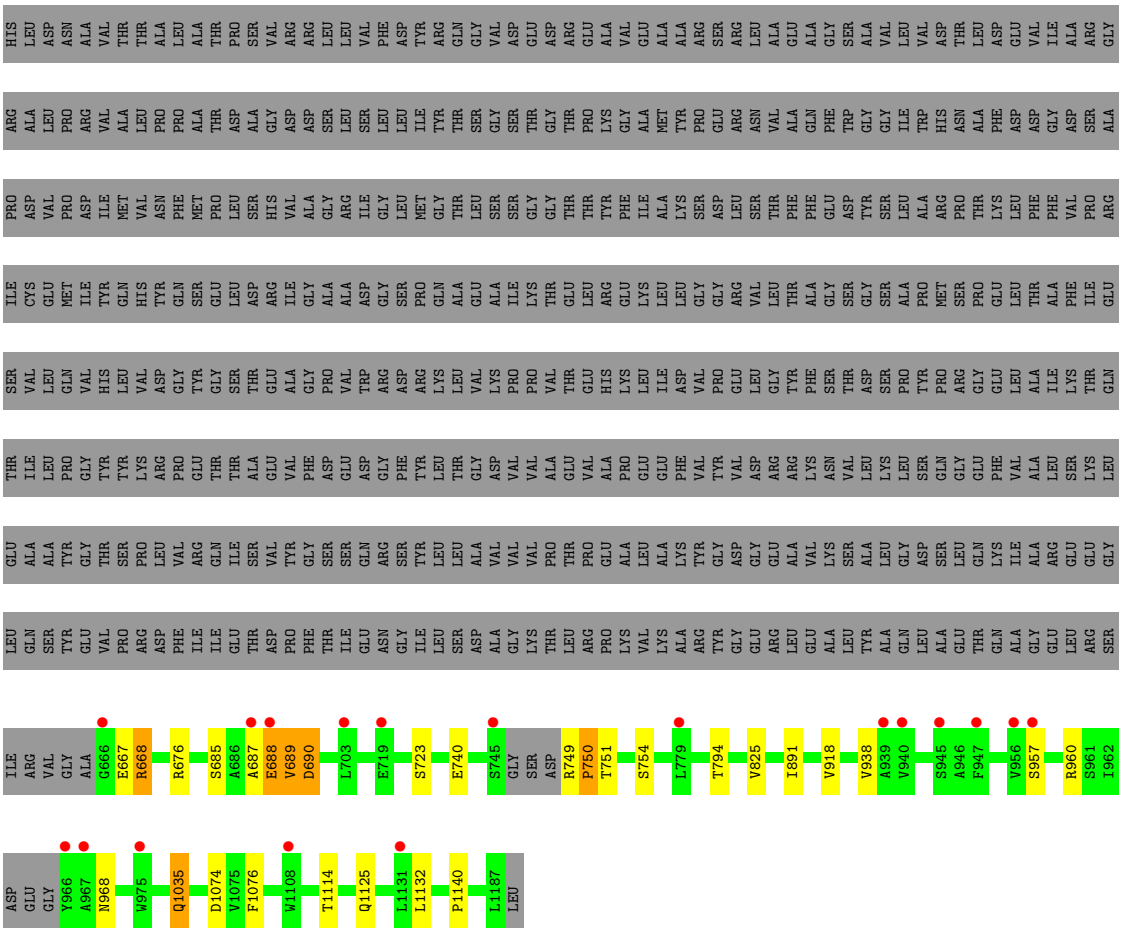
Chain B:

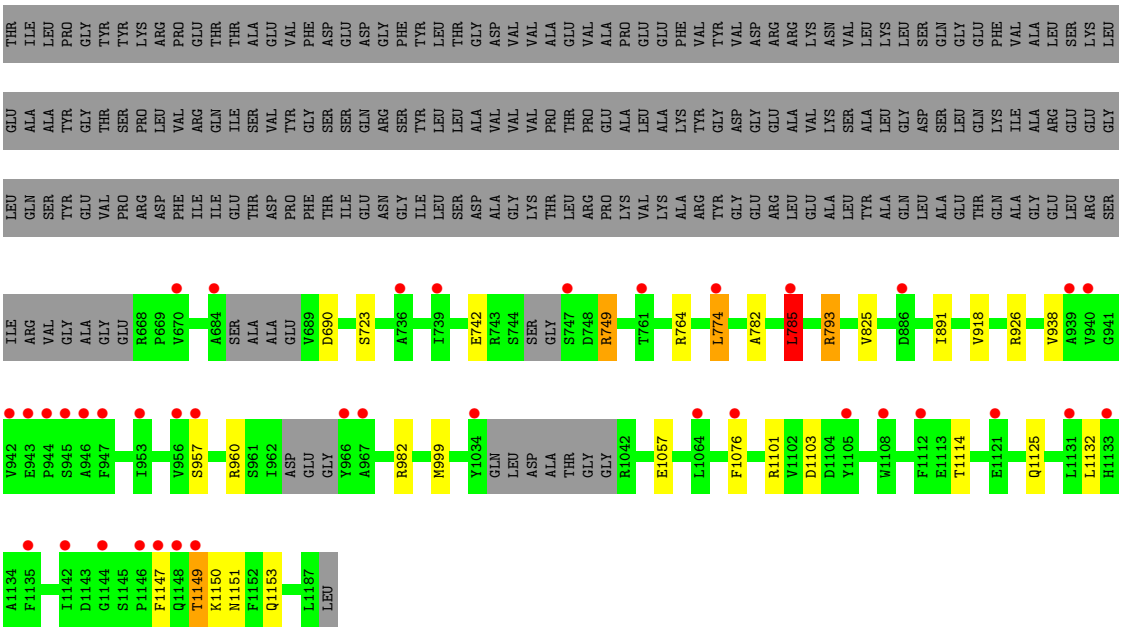


• Molecule 1: Thioester reductase domain-containing protein

Chain C:




HIS LEU ASP ASN ALA VAL THR THR ALA LEU ALA THR PRO SER VAL ARG ARG LEU LEU VAL PHE ASP TYR ARG GLN GLY VAL ASP GLU ASP ARG GLU ALA ALA ARG SER ARG LEU ALA GLU ALA GLY SER ALA VAL LEU VAL ASP THR LEU ASP GLU VAL ILE ALA ARG GLY
ARG ALA LEU PRO ARG VAL ALA LEU PRO PRO ALA THR ASP ALA GLY ASP ASP SER LEU SER LEU LEU ILE TYR THR SER GLY SER THR GLY GLY THR PRO LYS GLY ILE ALA MET TYR PRO GLU ARG ASN VAL ALA GLN PHE TRP GLY GLY ILE TRP HIS ASN ALA PHE ASP ASP GLY ASP SER ALA
PRO ASP VAL PRO ASP ILE MET VAL ASN PHE MET PRO LEU SER HIS VAL ALA GLY ARG ILE GLY LEU MET GLY THR LEU SER SER GLY GLY THR THR TYR PHE ILE ALA LYS SER ASP LEU SER THR PHE PHE GLU ASP TYR SER LEU ALA ARG PRO THR LYS LEU PHE PHE VAL PRO ARG
ILE CYS GLU MET ILE TYR GLN HIS TYR GLN SER GLU LEU ASP ARG ILE GLY ALA ALA ASP GLY SER PRO GLN ALA GLU ALA ILE LYS THR GLU LEU ARG GLU LYS LEU LEU GLY GLY ARG VAL LEU THR ALA GLY SER GLY SER ALA PRO MET SER PRO THR GLU LEU THR ALA PHE ILE GLU
SER VAL LEU GLN VAL HIS LEU VAL ASP GLY TYR GLY SER THR GLU ALA GLY PRO VAL TRP ARG ASP ARG LYS LEU VAL LYS PRO PRO VAL THR GLU HIS LYS LEU ILE ASP VAL PRO GLU LEU GLY TYR PHE SER THR ASP SER PRO TYR ARG ASP SER GLY LEU LYS LEU SER GLN LEU GLU GLN LEU ALA ILE LYS THR GLN
THR ILE LEU PRO GLY TYR TYR LYS ARG PRO GLU THR THR ALA GLU VAL PHE ASP GLU ASP GLY PHE TYR LEU THR GLY ASP VAL VAL ALA GLU VAL ALA PRO GLU GLU PHE VAL TYR VAL ASP ARG ARG LYS ASN VAL LEU LYS LEU SER GLN GLY GLU PHE VAL ALA LEU SER LYS LEU
GLU ALA ALA TYR GLY THR SER PRO LEU VAL ARG GLN ILE SER SER GLN ARG SER TYR LEU LEU ALA ALA VAL VAL PRO THR PRO GLU ALA LEU LYS TYR GLY SER GLU ALA ASP GLY GLU ALA VAL LYS SER ALA LEU GLY ASP SER LEU GLN LYS ILE ALA ARG GLU GLU GLY
LEU GLN SER TYR GLU VAL PRO ARG ASP PHE ILE ILE GLU THR ASP PRO PHE THR ILE GLU ASN GLY ILE LEU SER ASP ALA GLY LYS THR LEU ARG PRO LYS VAL LYS ALA ARG TYR GLY GLU ARG LEU GLU ALA LEU TYR ALA GLN LEU ALA GLY GLU SER ARG SER
ILE ARG VAL GLY ALA GLU ASP ASP ASP


THR ILE LEU PRO GLY TYR TYR LYS ARG PRO GLU THR THR ALA GLU VAL PHE ASP GLU ASP GLY PHE TYR LEU THR GLY ASP VAL VAL ALA GLU VAL ALA PRO GLU GLU PHE VAL TYR VAL ASP ARG ARG LYS ASN VAL LEU LYS LEU SER GLN GLY GLU PHE VAL ALA LEU SER LYS LEU
GLU ALA ALA TYR GLY THR SER PRO LEU VAL ARG GLN ILE SER VAL TYR GLY SER SER GLN ARG SER TYR LEU LEU ALA VAL VAL VAL PRO THR PRO GLU ALA LEU ALA LYS TYR GLY ASP GLY GLU ALA VAL LYS SER ALA LEU GLY ASP SER LEU GLN LYS ILE ALA ARG GLU GLU GLY
LEU GLN SER TYR GLU VAL PRO ARG ASP PHE ILE ILE GLU THR ASP PRO PHE THR ILE GLU ASN GLY ILE LEU SER ASP ALA GLY LYS THR LEU ARG PRO LYS VAL LYS ALA ARG TYR GLY GLU ARG LEU GLU ALA LEU TYR ALA GLN LEU GLY ALA LEU GLU THR GLN ALA ILE GLY GLU LEU GLU ARG SER
ILE ARG VAL GLY ALA GLY GLU R668 P669 V670 A684 SER ALA ALA GLU V689 D690 S723 A736 I739 E742 R743 S744 SER GLY S747 D748 R749 T761 R764 L774 A782 L785 R793 V825 D886 I891 V918 R926 V938 A939 V940 G941
V942 E943 P944 S945 A946 F947 I963 V956 S957 R960 S961 I962 ASP GLU GLY Y966 A967 R982 M999 Y1034 GLN LEU ASP ALA THR GLY GLY R1042 E1057 L1064 F1076 R1101 V1102 D1103 D1104 Y1105 W1108 F1112 E1113 T1114 E1121 Q1125 L1131 L1132 H1133
A1134 F1135 I1142 D1143 G1144 S1145 P1146 F1147 Q1148 T1149 K1150 N1151 F1152 Q1153 L1187 LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	94.94Å 94.94Å 335.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	200.00 – 2.37 91.36 – 2.37	Depositor EDS
% Data completeness (in resolution range)	98.7 (200.00-2.37) 98.7 (91.36-2.37)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.219 , 0.241 0.229 , 0.245	Depositor DCC
R_{free} test set	5667 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	50.2	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 40.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.057 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16105	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.41	0/4011	0.65	2/5457 (0.0%)
1	B	0.41	0/4060	0.69	5/5525 (0.1%)
1	C	0.41	0/4030	0.67	3/5483 (0.1%)
1	D	0.42	0/3953	0.69	10/5376 (0.2%)
All	All	0.41	0/16054	0.67	20/21841 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	733	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	B	733	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	D	793	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	D	764	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	D	1101	ARG	NE-CZ-NH1	6.78	123.69	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	924	THR	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3926	0	3880	5	0
1	B	3973	0	3912	4	1
1	C	3944	0	3894	9	1
1	D	3869	0	3825	15	0
2	A	40	0	19	0	0
2	B	40	0	19	0	0
2	C	40	0	19	0	0
2	D	40	0	19	0	0
3	A	63	0	0	0	0
3	B	75	0	0	0	0
3	C	58	0	0	0	0
3	D	37	0	0	0	0
All	All	16105	0	15587	33	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 33 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:782:ALA:HA	1:D:785:LEU:HD12	1.57	0.86
1:C:750:PRO:O	1:C:754:SER:OG	2.05	0.75
1:D:785:LEU:HD23	1:D:926:ARG:HA	1.67	0.74
1:A:667:GLU:HB2	1:A:668:ARG:HB2	1.75	0.69
1:D:1076:PHE:CE1	1:D:1149:THR:OG1	2.46	0.68

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:925:LYS:NZ	1:C:740:GLU:OE1[3_664]	2.14	0.06

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	508/1188 (43%)	491 (97%)	15 (3%)	2 (0%)	34	46
1	B	516/1188 (43%)	499 (97%)	15 (3%)	2 (0%)	34	46
1	C	510/1188 (43%)	490 (96%)	18 (4%)	2 (0%)	34	46
1	D	494/1188 (42%)	477 (97%)	14 (3%)	3 (1%)	25	34
All	All	2028/4752 (43%)	1957 (96%)	62 (3%)	9 (0%)	34	46

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	668	ARG
1	B	668	ARG
1	B	749	ARG
1	C	668	ARG
1	D	690	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	409/947 (43%)	399 (98%)	10 (2%)	49	66
1	B	414/947 (44%)	399 (96%)	15 (4%)	35	51
1	C	411/947 (43%)	398 (97%)	13 (3%)	39	56
1	D	405/947 (43%)	392 (97%)	13 (3%)	39	56
All	All	1639/3788 (43%)	1588 (97%)	51 (3%)	40	57

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	723	SER
1	C	1114	THR
1	D	1125	GLN
1	C	749	ARG
1	C	957	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	675	GLN
1	C	1011	ASN
1	D	675	GLN
1	C	1157	GLN
1	B	1126	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAP	D	1201	-	36,43,52	0.87	2 (5%)	44,67,80	1.29	6 (13%)
2	NAP	C	1201	-	36,43,52	0.92	2 (5%)	44,67,80	1.24	4 (9%)
2	NAP	A	1201	-	36,43,52	0.90	2 (5%)	44,67,80	1.22	4 (9%)
2	NAP	B	1201	-	36,43,52	0.89	2 (5%)	44,67,80	1.16	3 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	D	1201	-	-	4/23/59/67	0/4/4/5
2	NAP	C	1201	-	-	5/23/59/67	0/4/4/5
2	NAP	A	1201	-	-	4/23/59/67	0/4/4/5
2	NAP	B	1201	-	-	5/23/59/67	0/4/4/5

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1201	NAP	C5A-C4A	2.48	1.47	1.40
2	A	1201	NAP	C5A-C4A	2.42	1.47	1.40
2	D	1201	NAP	C5A-C4A	2.37	1.47	1.40
2	B	1201	NAP	C2A-N3A	2.34	1.35	1.32
2	B	1201	NAP	C5A-C4A	2.34	1.47	1.40

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1201	NAP	N3A-C2A-N1A	-4.14	122.21	128.68
2	B	1201	NAP	N3A-C2A-N1A	-3.99	122.44	128.68
2	C	1201	NAP	N3A-C2A-N1A	-3.89	122.59	128.68
2	A	1201	NAP	N3A-C2A-N1A	-3.74	122.84	128.68
2	C	1201	NAP	PN-O3-PA	-2.94	122.75	132.83

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	NAP	C5D-O5D-PN-O2N
2	B	1201	NAP	C5D-O5D-PN-O1N

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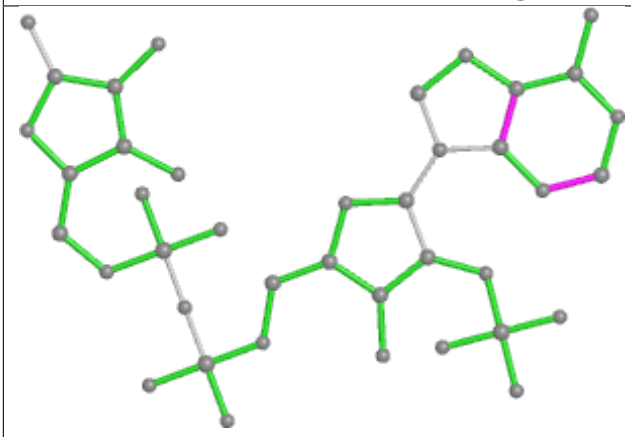
Mol	Chain	Res	Type	Atoms
2	B	1201	NAP	C5D-O5D-PN-O2N
2	C	1201	NAP	C5D-O5D-PN-O1N
2	C	1201	NAP	C5D-O5D-PN-O2N

There are no ring outliers.

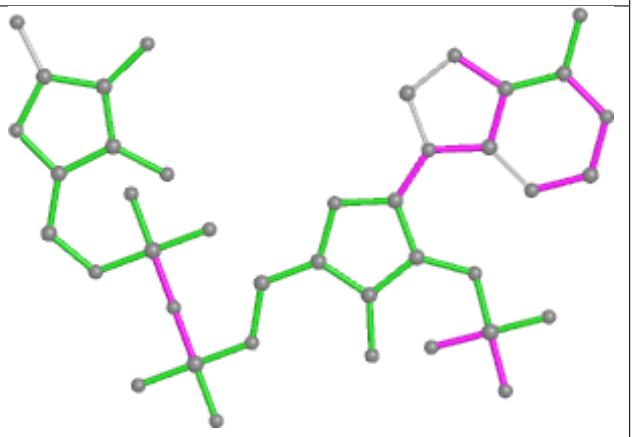
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

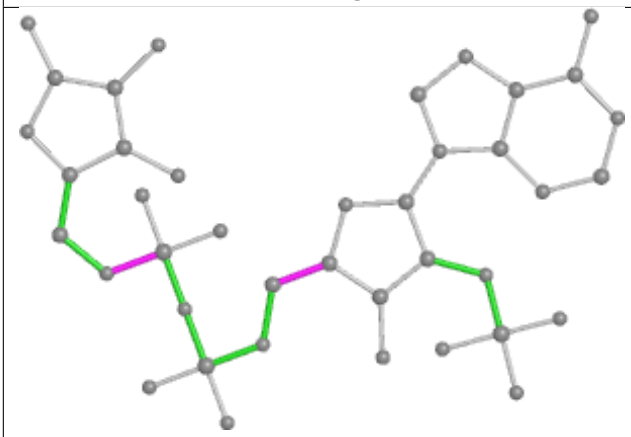
Ligand NAP D 1201



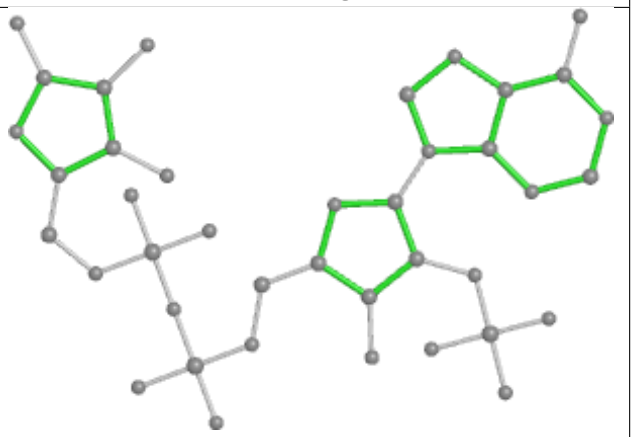
Bond lengths



Bond angles

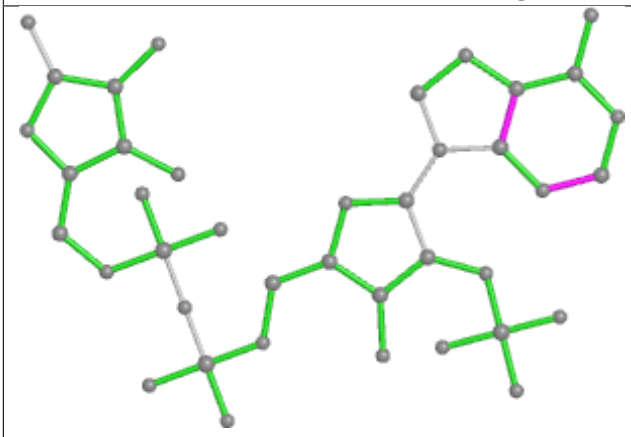


Torsions

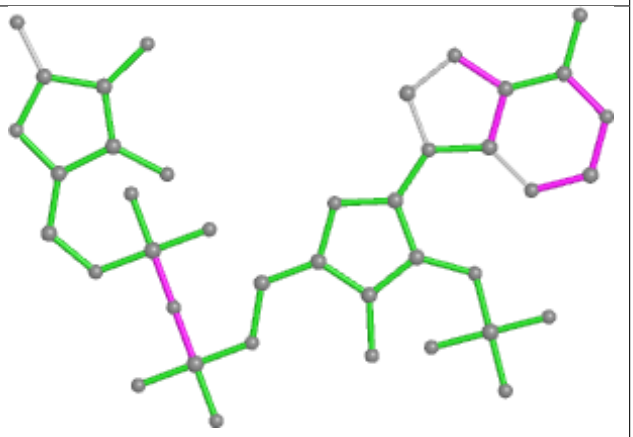


Rings

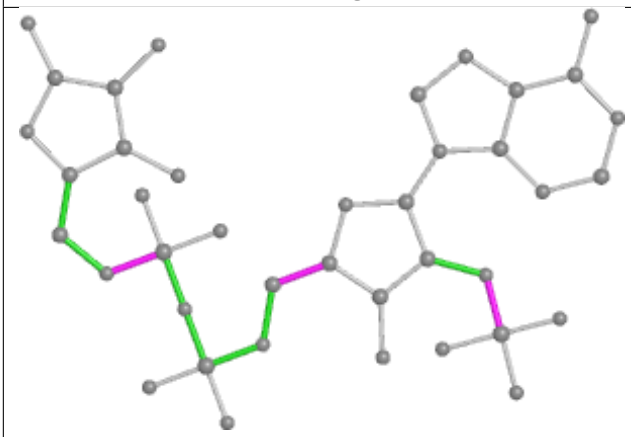
Ligand NAP C 1201



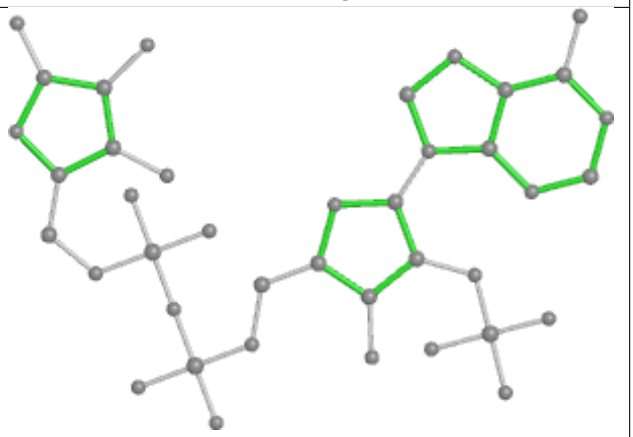
Bond lengths



Bond angles

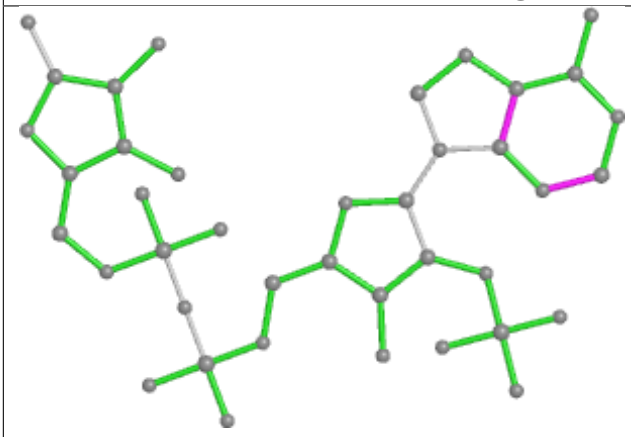


Torsions

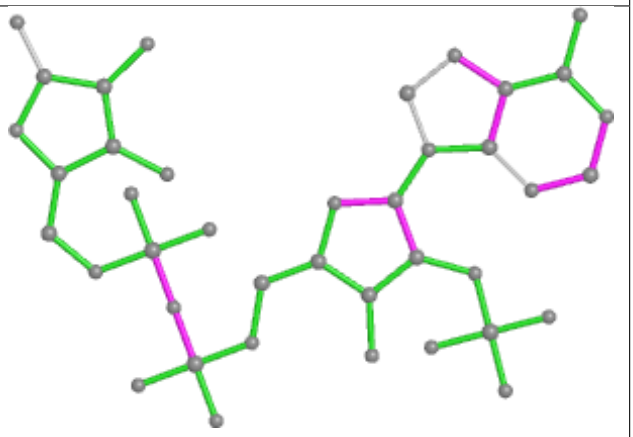


Rings

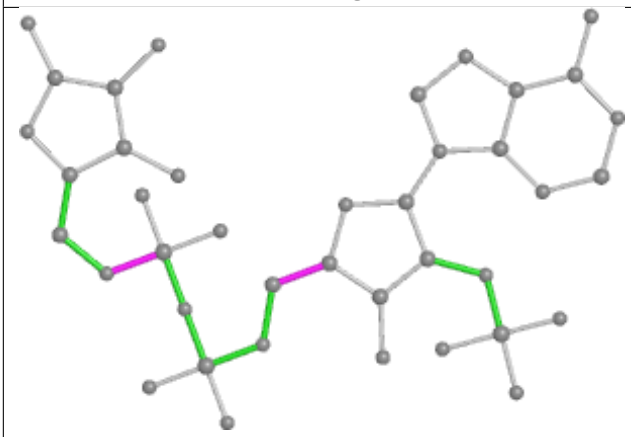
Ligand NAP A 1201



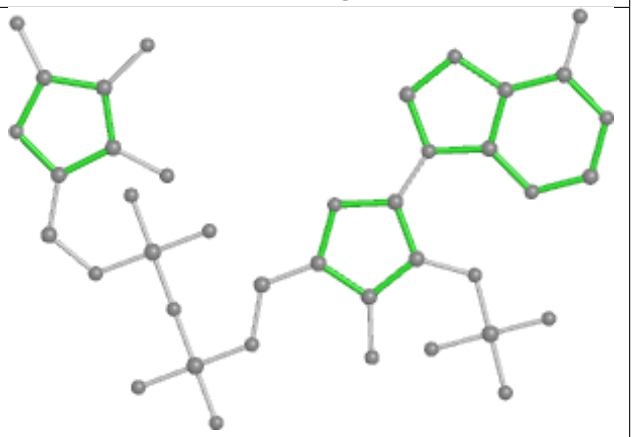
Bond lengths



Bond angles

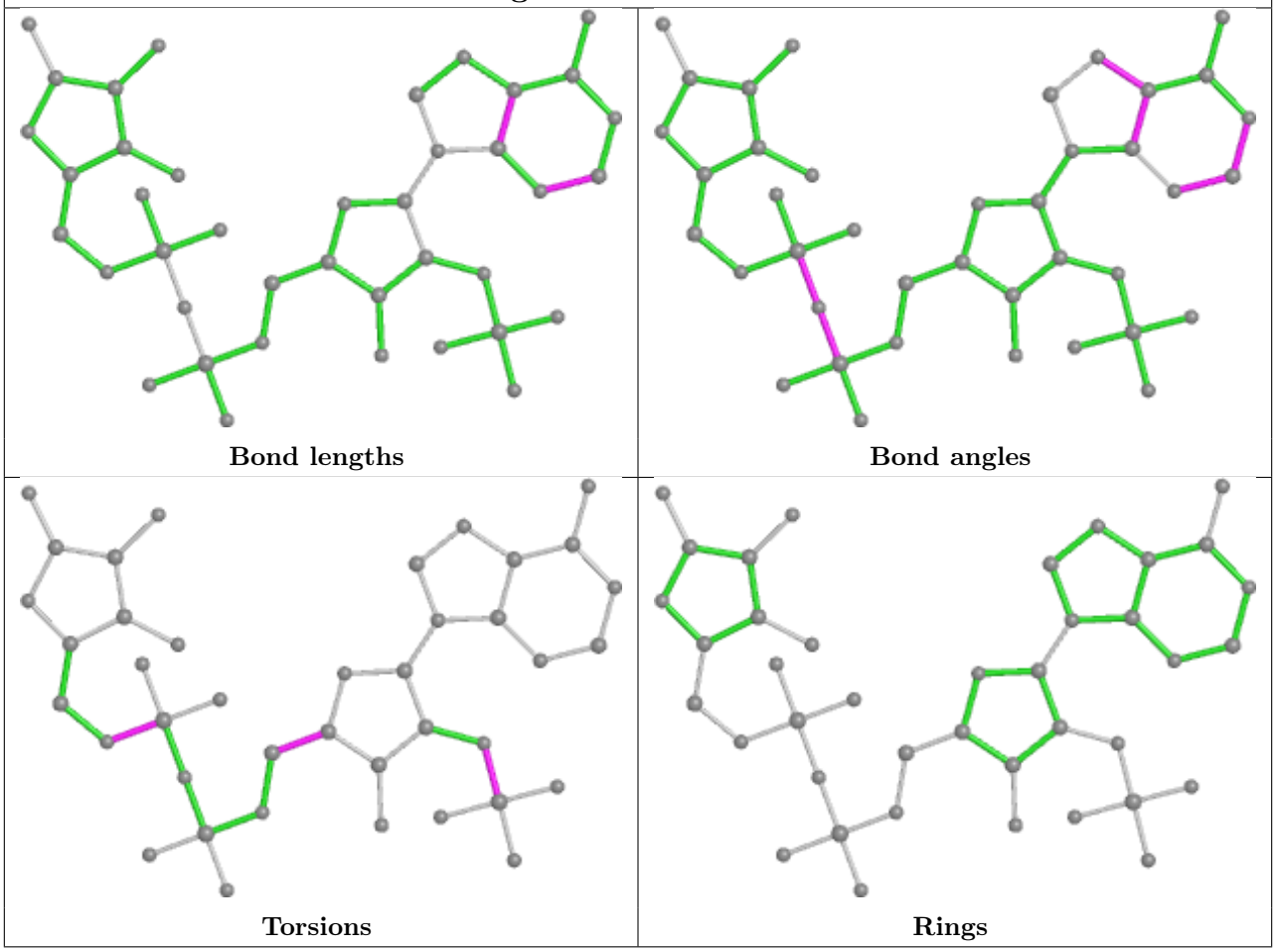


Torsions



Rings

Ligand NAP B 1201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	514/1188 (43%)	0.36	11 (2%)	63	65	44, 79, 126, 182	0
1	B	520/1188 (43%)	0.34	10 (1%)	66	68	42, 75, 126, 187	0
1	C	516/1188 (43%)	0.49	18 (3%)	44	47	41, 84, 141, 203	0
1	D	504/1188 (42%)	0.78	38 (7%)	14	15	46, 93, 153, 185	0
All	All	2054/4752 (43%)	0.49	77 (3%)	41	45	41, 82, 142, 203	0

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	966	TYR	7.3
1	D	945	SER	6.9
1	D	1146	PRO	6.7
1	C	687	ALA	6.7
1	D	966	TYR	6.5

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

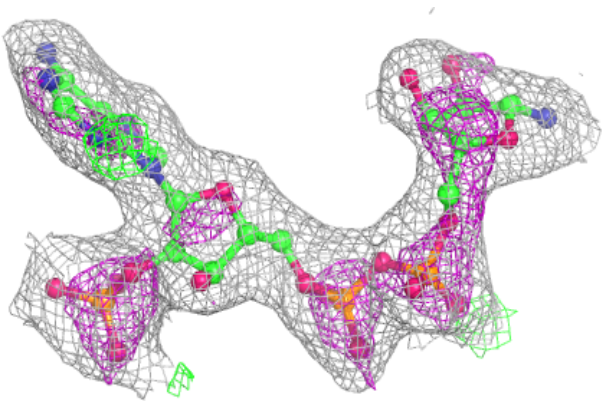
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

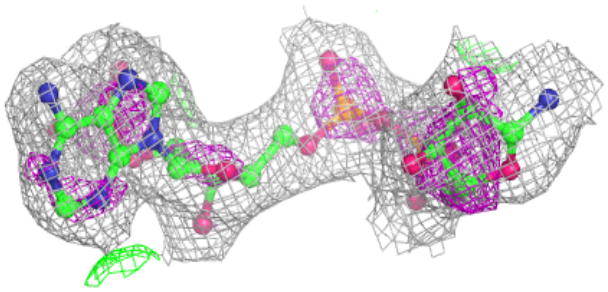
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAP	D	1201	40/48	0.97	0.12	37,42,66,68	0
2	NAP	B	1201	40/48	0.98	0.10	34,43,61,61	0
2	NAP	C	1201	40/48	0.98	0.12	37,44,65,67	0
2	NAP	A	1201	40/48	0.98	0.11	37,43,60,60	0

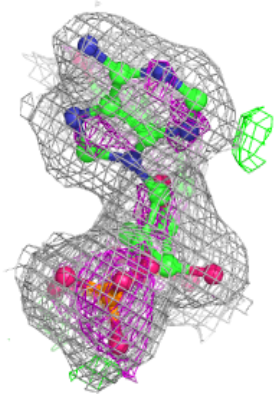
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAP D 1201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

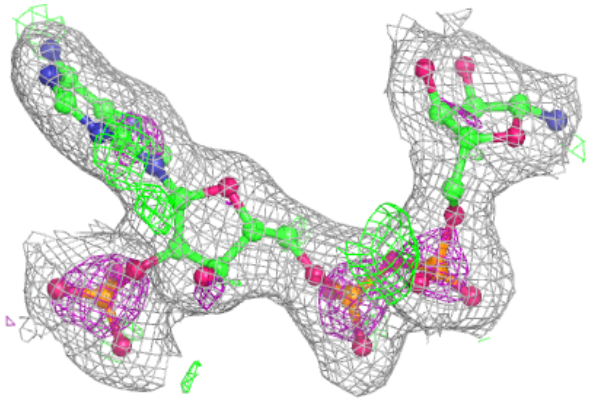


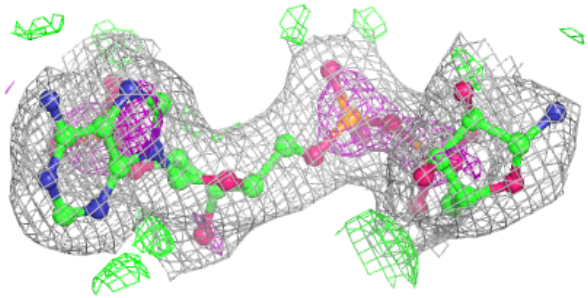


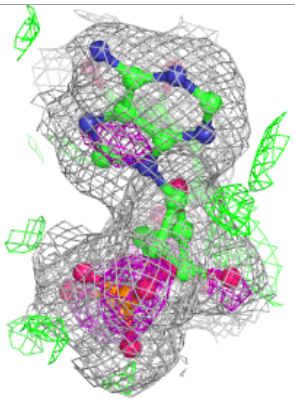


Electron density around NAP B 1201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

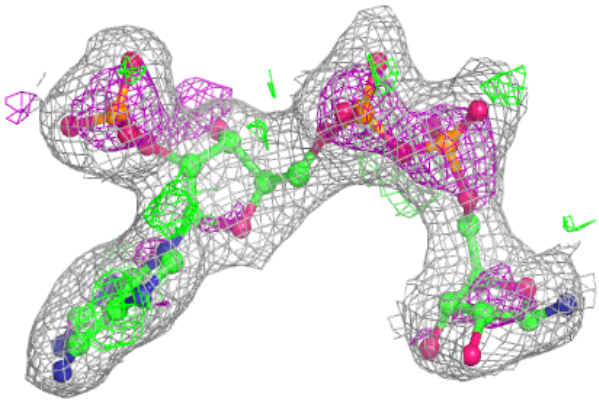


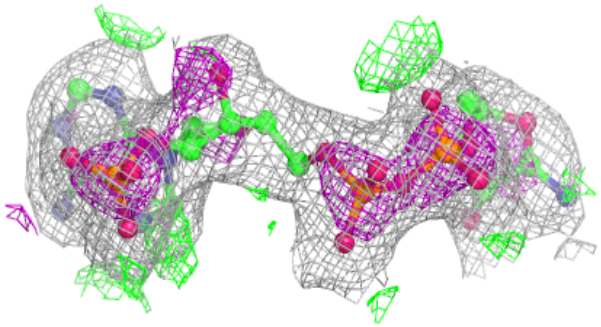


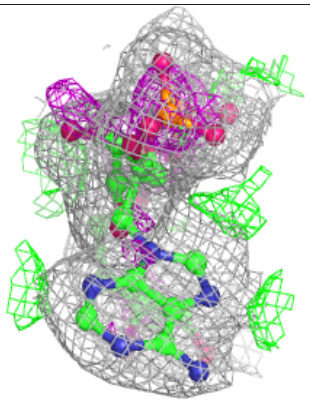


Electron density around NAP C 1201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

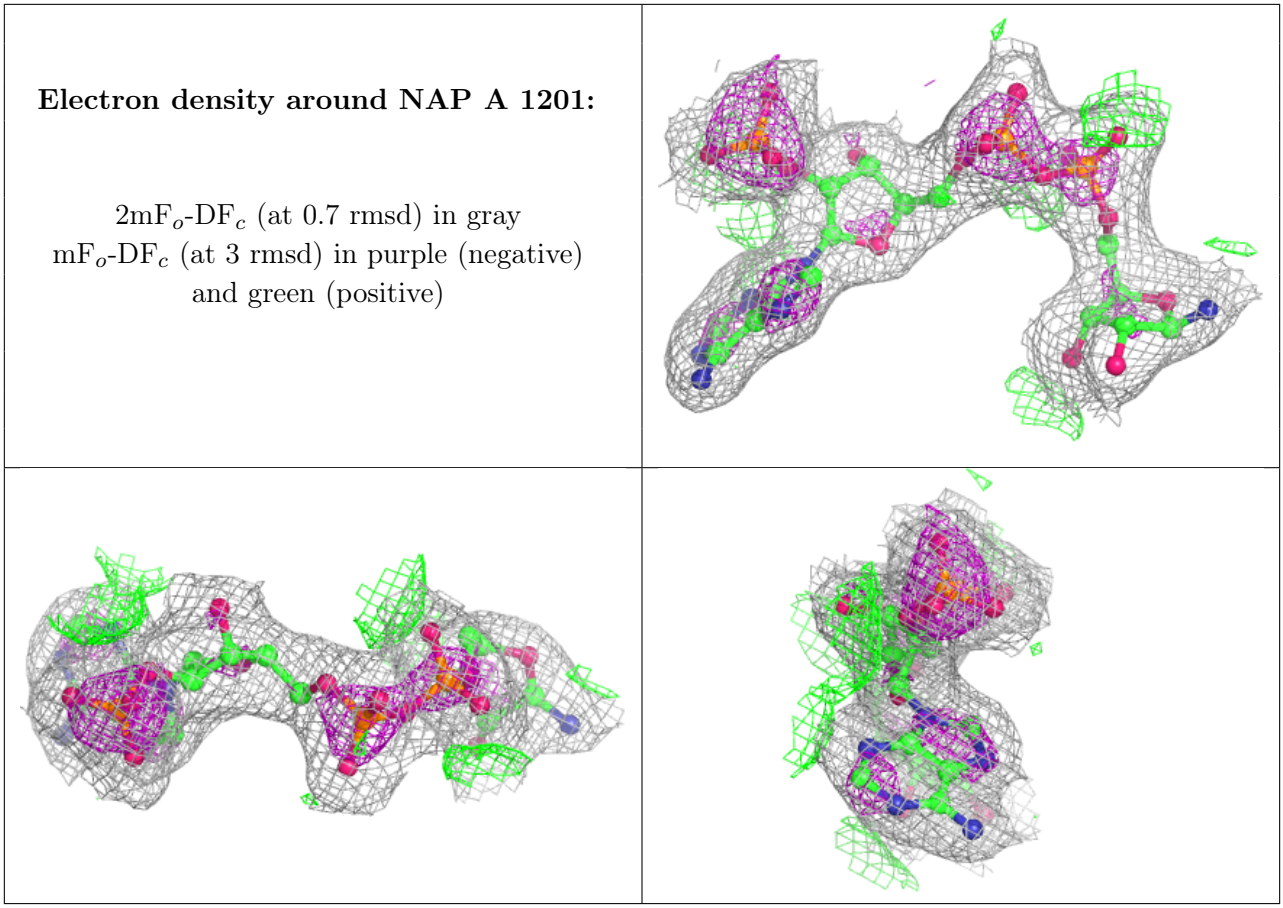






Electron density around NAP A 1201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.